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Kubik, Stefan; Goddard, Richard; Otto, Sijbren; Pohl, Susanne; Reyheller, Carsten; Stüwe, Sabine

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Optimization of the binding properties of a synthetic anion receptor using rational and combinatorial strategies

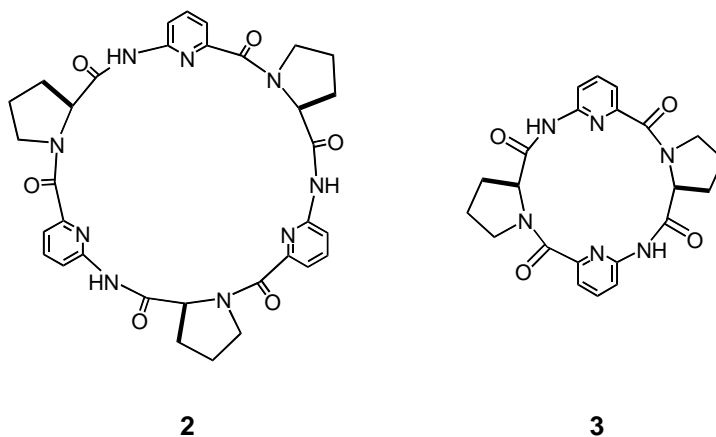
Stefan Kubik^{a,*}, Richard Goddard^b, Sijbren Otto^c, Susanne Pohl^a, Carsten Reyheller^a, Sabine Stüwe^a

^a *Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität, Universitätsstr. 1, D-40225 Düsseldorf, Germany, Email: kubik@uni-duesseldorf.de*

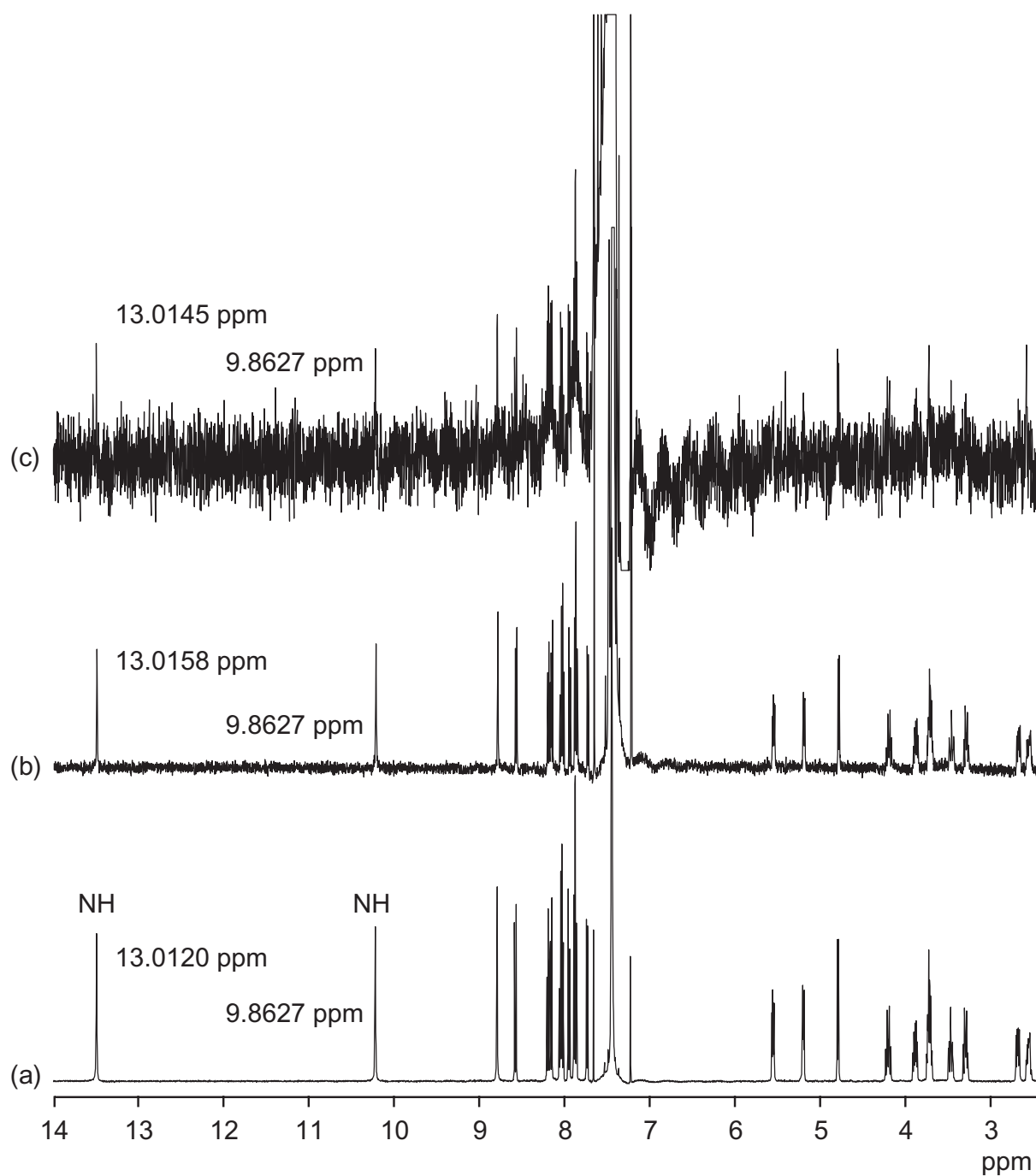
^b *Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470 Mülheim/Ruhr, Germany*

^c *Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, U.K.*

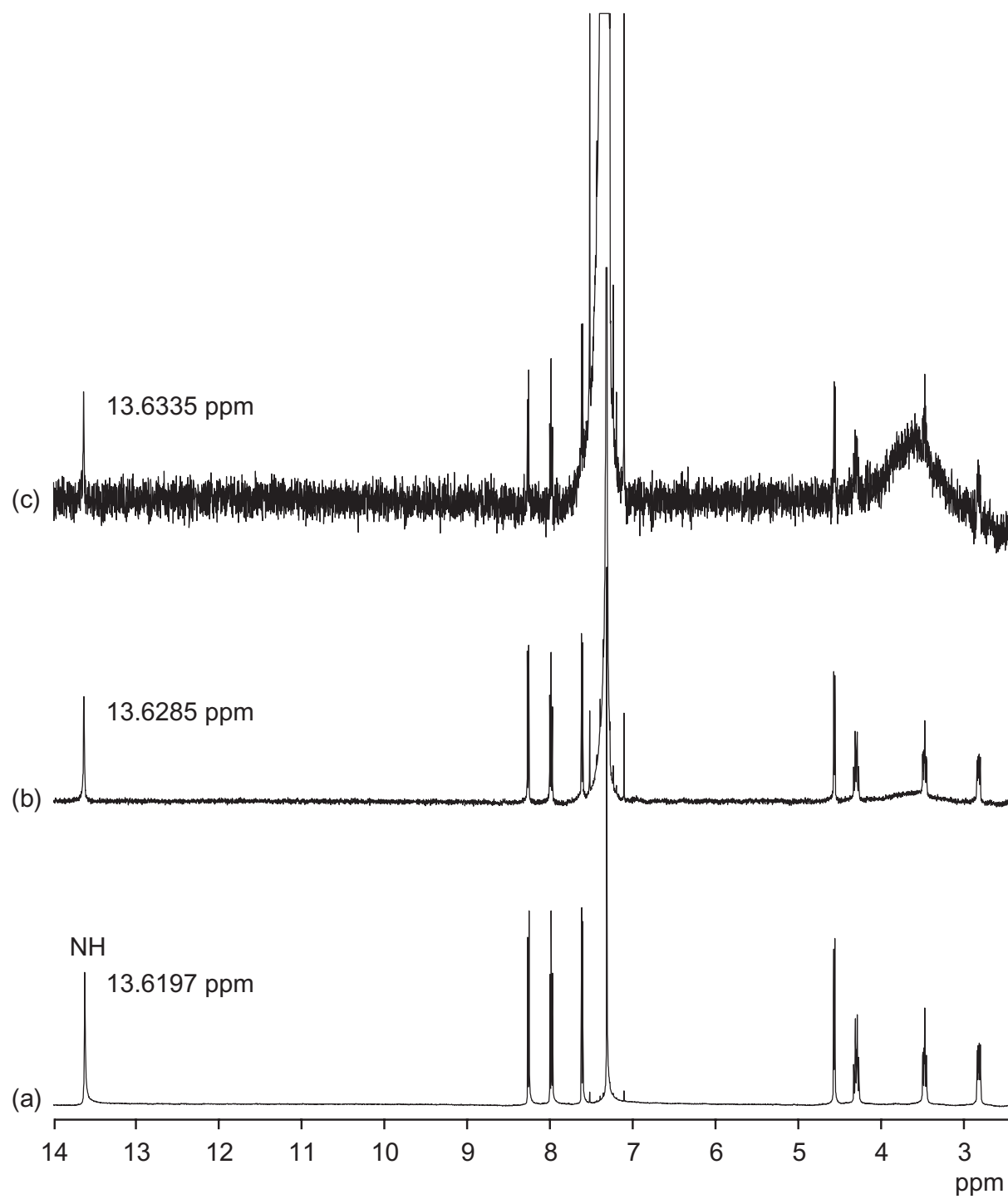
Structure of compounds **2** and **3**:



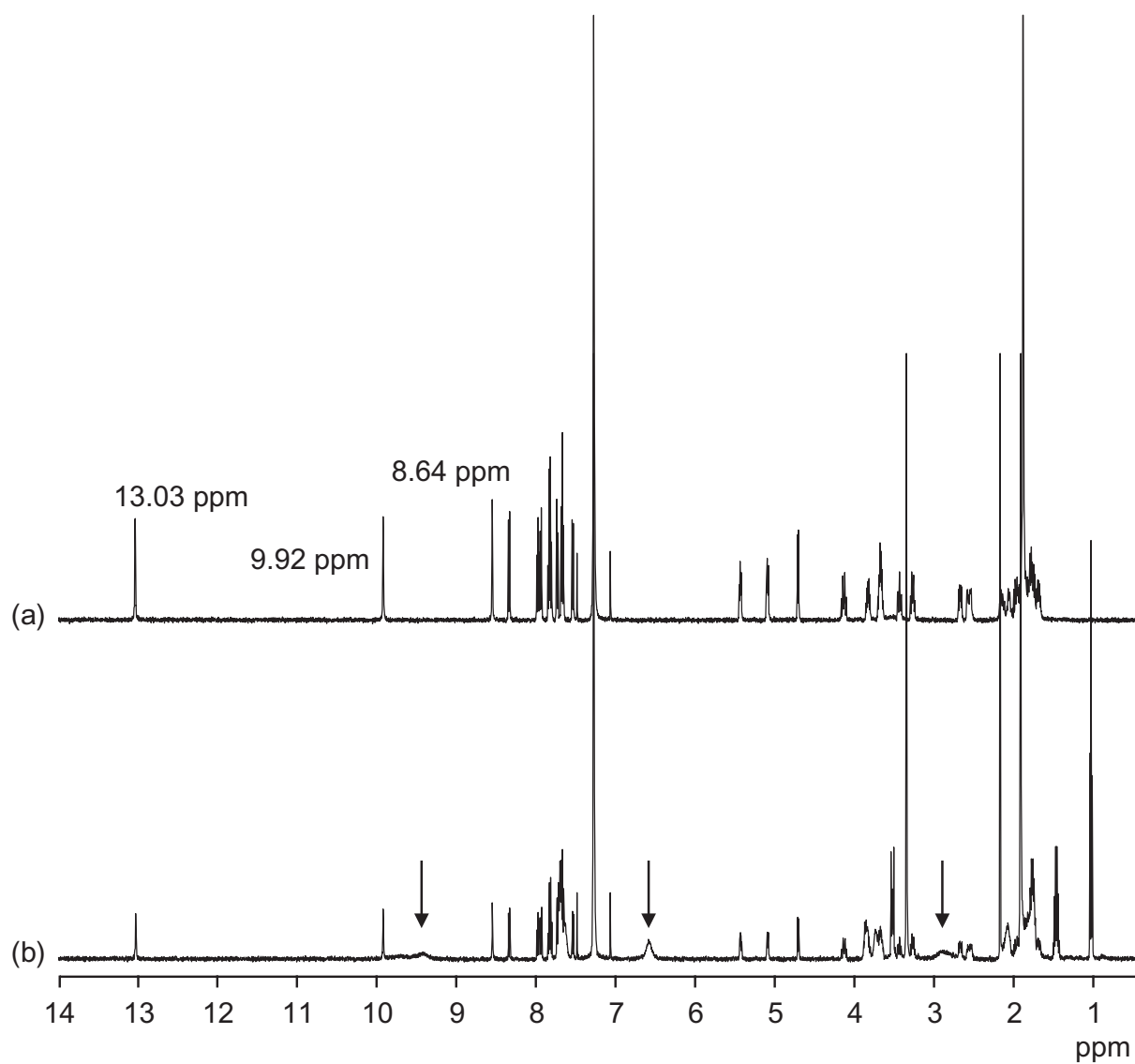
Concentration-dependent NMR spectra: 2 in CDCl₃ (a) 2 mM, (b) 0.2 mM, (c) 0.02 mM (Bruker DRX 500 / 500 MHz)



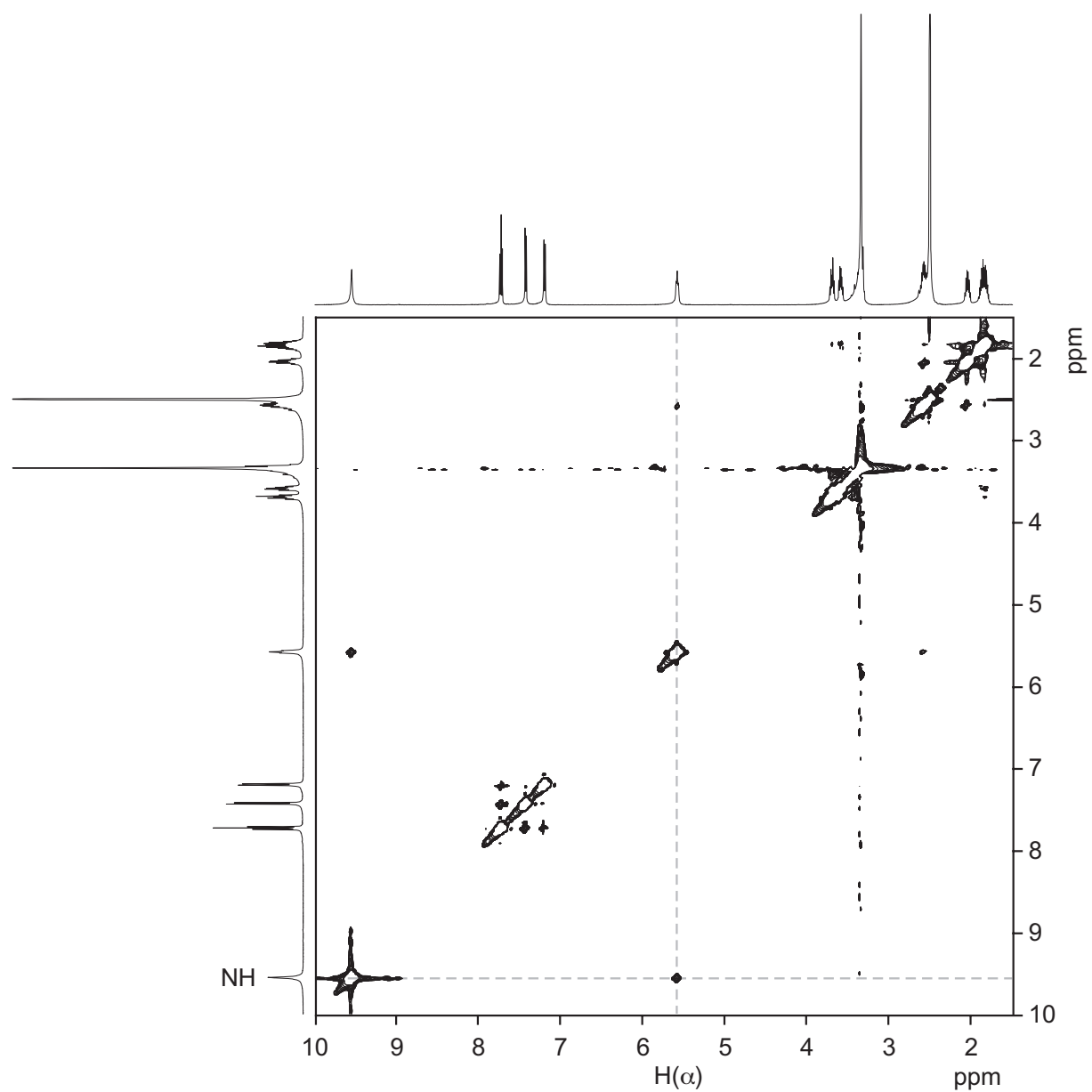
Concentration-dependent NMR spectra: 3 in CDCl₃ (a) 2 mM, (b) 0.2 mM, (c) 0.02 mM (Bruker DRX 500 / 500 MHz)



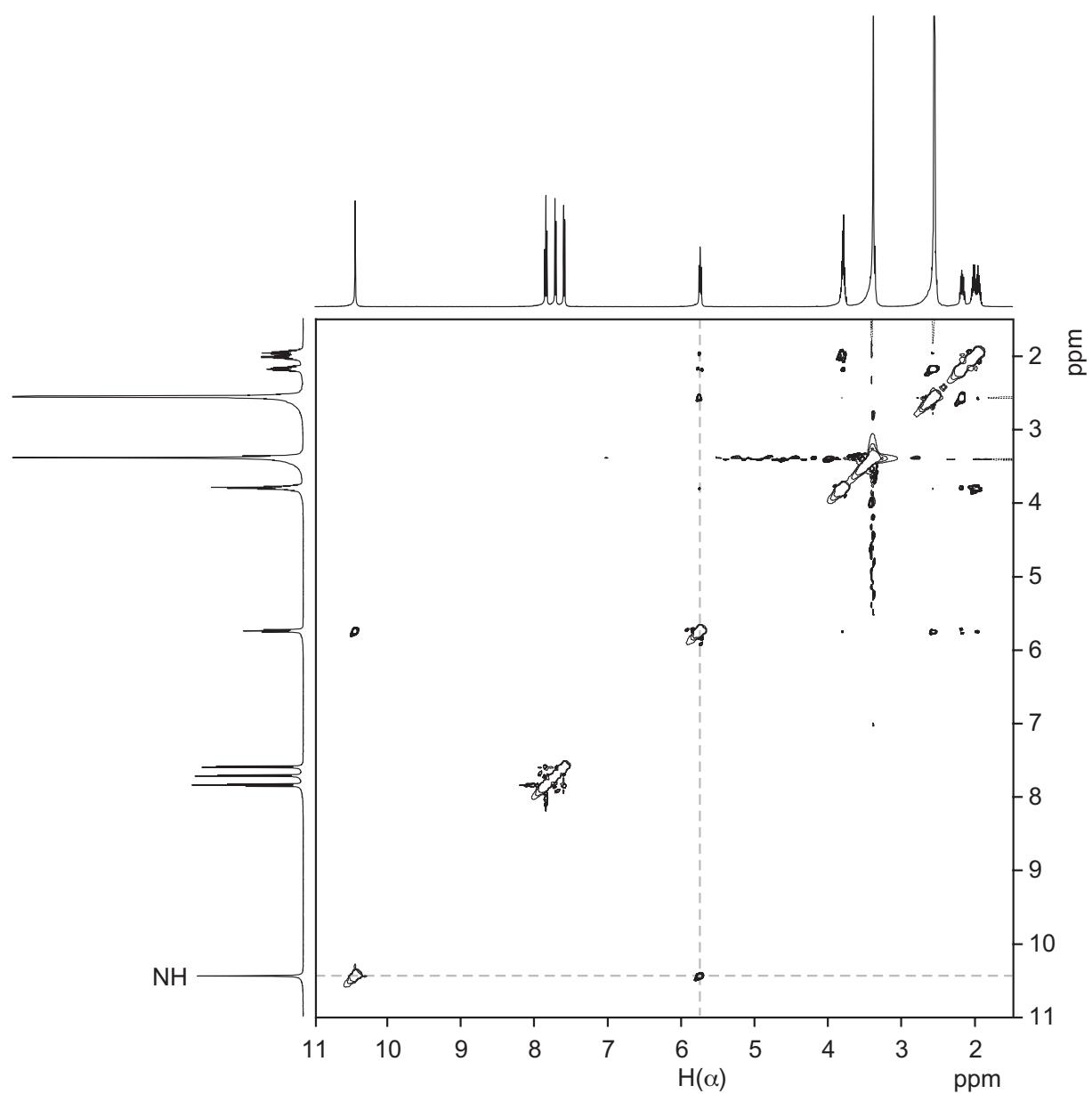
¹H-NMR spectra: **2** (1 mM) in CDCl₃ (a), **2** (1 mM) + 1 equiv of *n*-butyltrimethylammonium iodide in CDCl₃ (b).



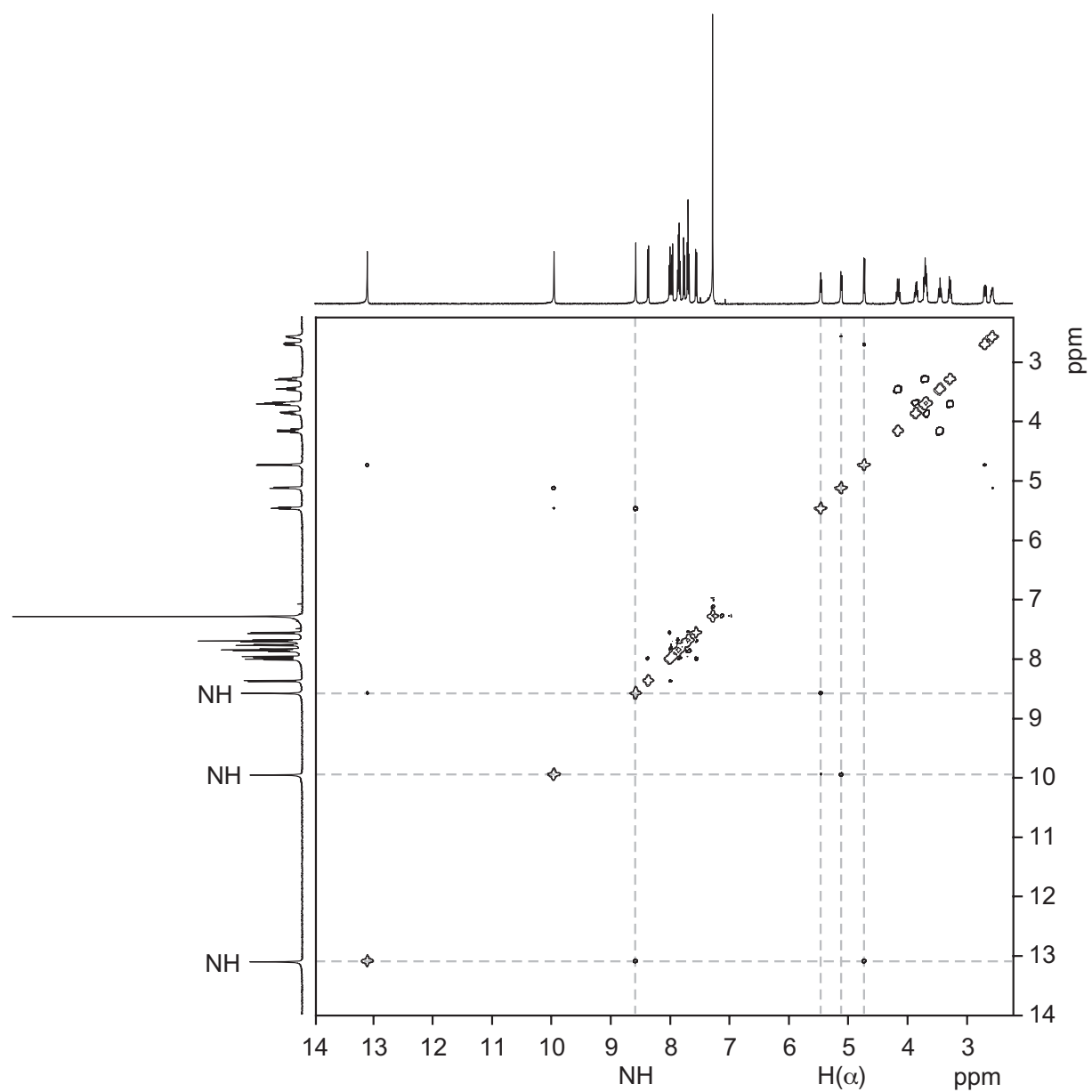
NOESY NMR spectrum: 2 (1 mM) in d_6 -DMSO (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



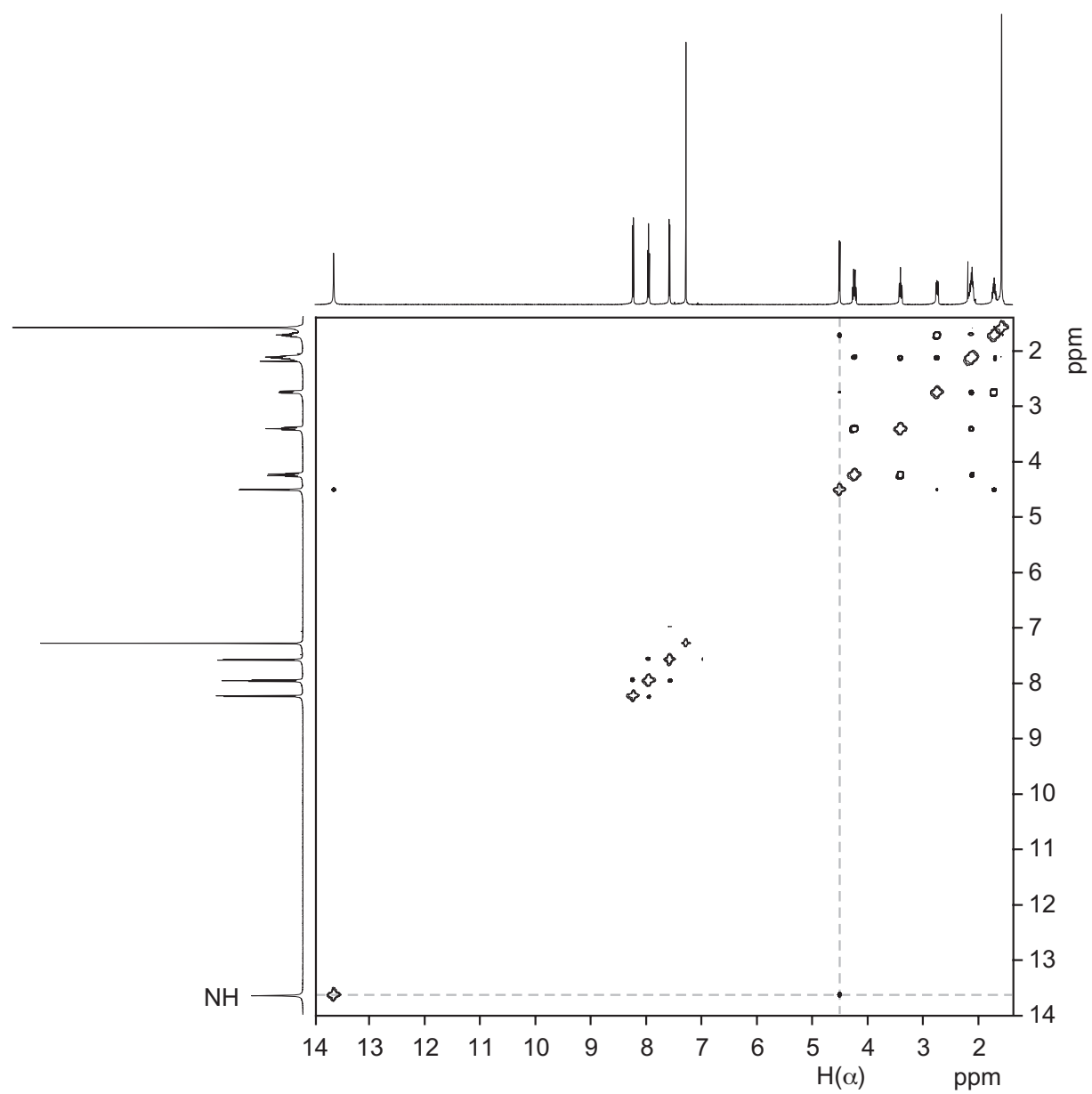
NOESY NMR spectrum: 3 (1 mM) in d_6 -DMSO (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



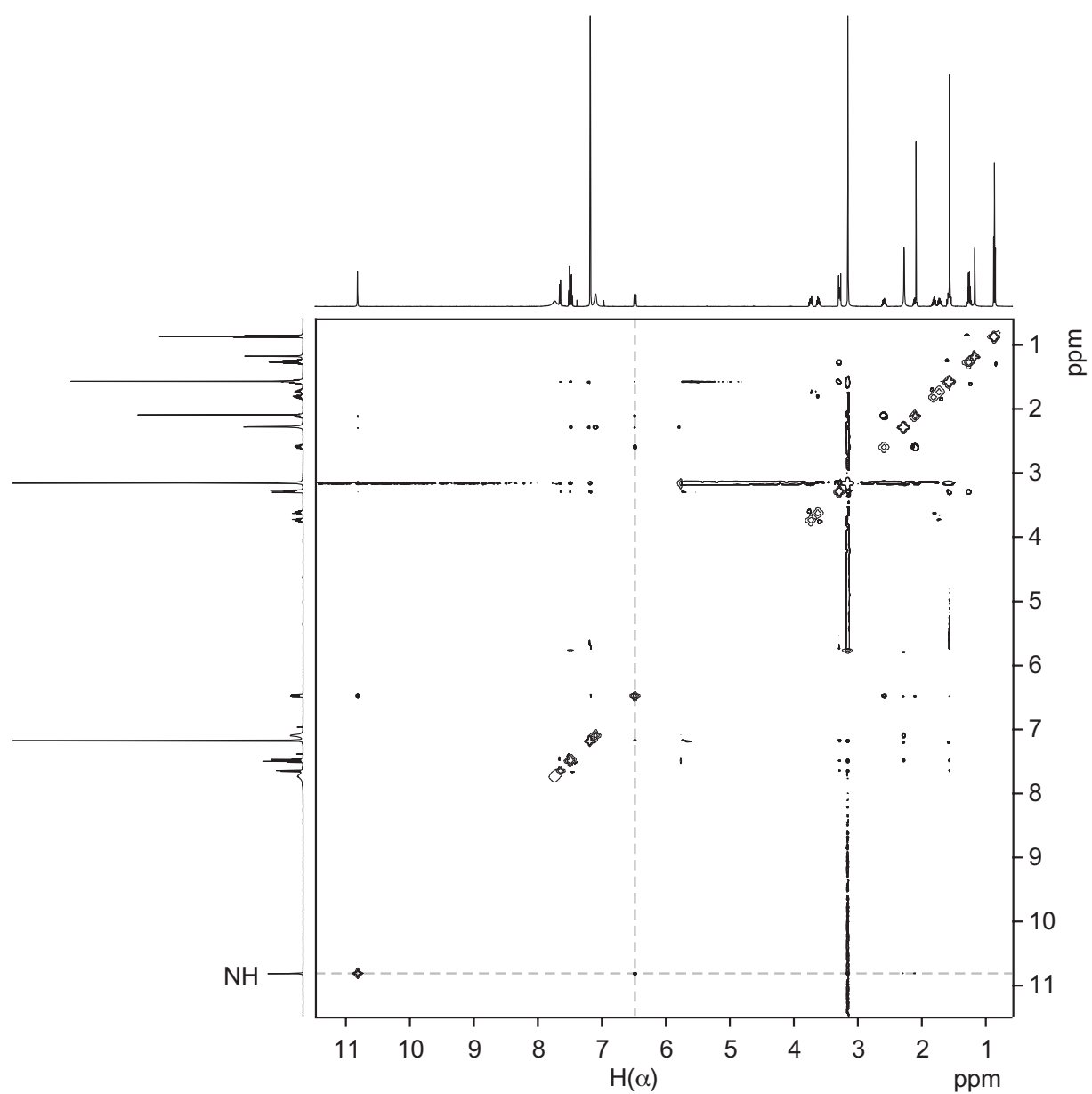
NOESY NMR spectrum: **2** (1 mM) in CDCl₃ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



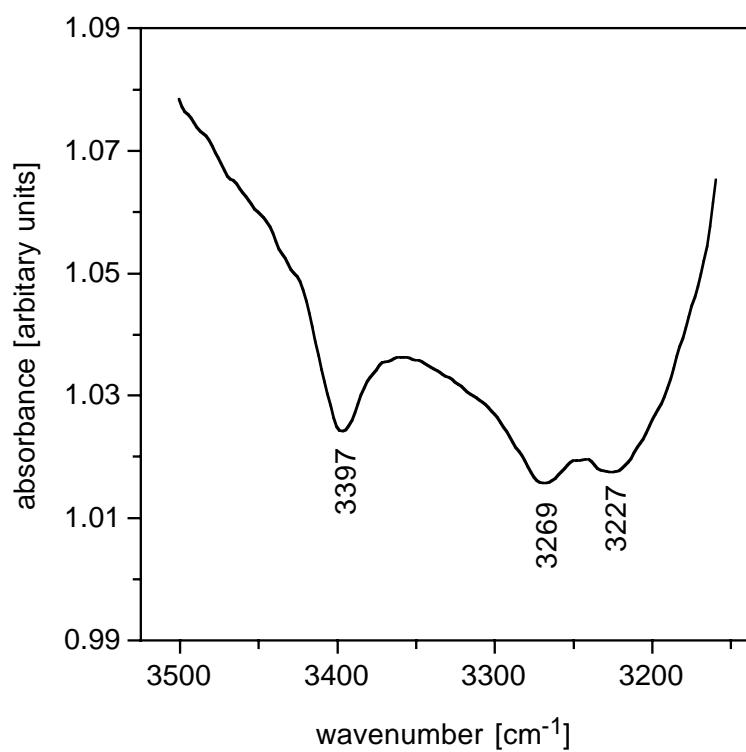
NOESY NMR spectrum: **3** (1 mM) in CDCl₃ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



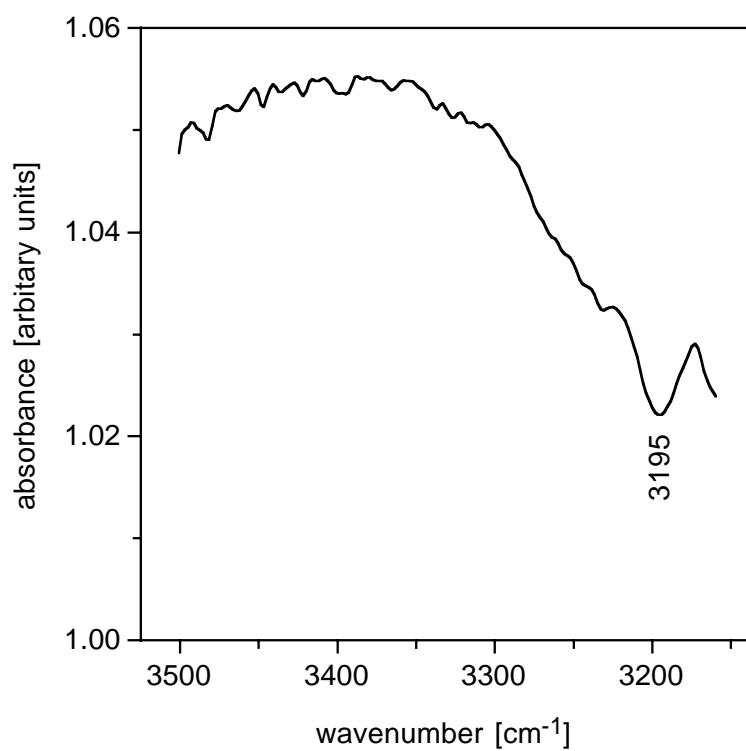
NOESY NMR spectrum: **2** (1 mM) after the addition of 3 equiv. of *n*-butyltrimethylammonium tosylate in CDCl₃ (mixing time 300 ms) (Bruker DRX 500 / 500 MHz).



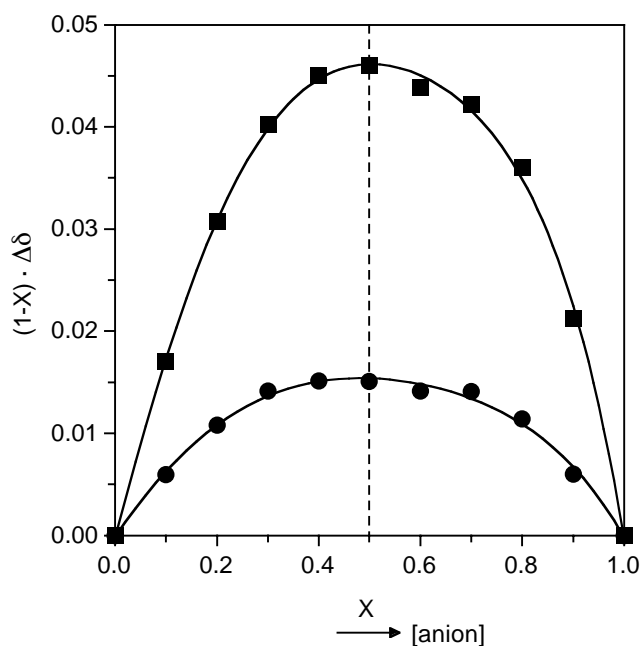
FT-IR spectrum: 2 in 1% [d₆]DMSO/CDCl₃ (c = 2mM)



FT-IR spectrum: 3 in CDCl₃ (c = 2mM)



Job-Plot: **2** + *n*-butyltrimethylammonium iodide in *d*₆-DMSO ($\Delta\delta$ = variation of the shift of the ProH(α) (squares) and the APAH(3) signal (circles) of **2**).



NMR Titration: Experimental (circles, squares) and calculated (line) saturation curves for the complex formation between **2** and *n*-butyltrimethylammonium iodide in *d*₆-DMSO ($\Delta\delta$ = variation of the shift of the ProH(α) (squares) and the APAH(3) signal (circles) of **2**)

